PUBCHEM_54605649

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 6.14e-01

Global applicability domain: Inside

Local applicability domain index: 2.46e-01

Confidence level: 8.72e-01

Nearest Neighbors from the Training Set

Image not found
2-Amino-5-methylbenzenesulfonic acid
Measured: 0.6
Predicted: 7.98e-01

Image not found
Sodium 3-nitrobenzenesulfonate
Measured: 0.7
Predicted: 7.21e-01

Image not found
4-Amino-1-naphthalenesulfonic acid sodium salt
Measured: 0.78
Predicted: 7.49e-01

Image not found
7-Amino-4-hydroxynaphthalene-2-sulfonic acid
Measured: 0.38
Predicted: 6.78e-01

Image not found
6-Amino-4-hydroxynaphthalene-2-sulfonic acid
Measured: 0.61
Predicted: 6.78e-01